



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 27, 2023 – 01:51 PM EDT

PDB ID : 3H0M  
Title : Structure of trna-dependent amidotransferase gatcab from aquifex aeolicus  
Authors : Wu, J.; Bu, W.; Sheppard, K.; Kitabatake, M.; Soll, D.; Smith, J.L.  
Deposited on : 2009-04-09  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

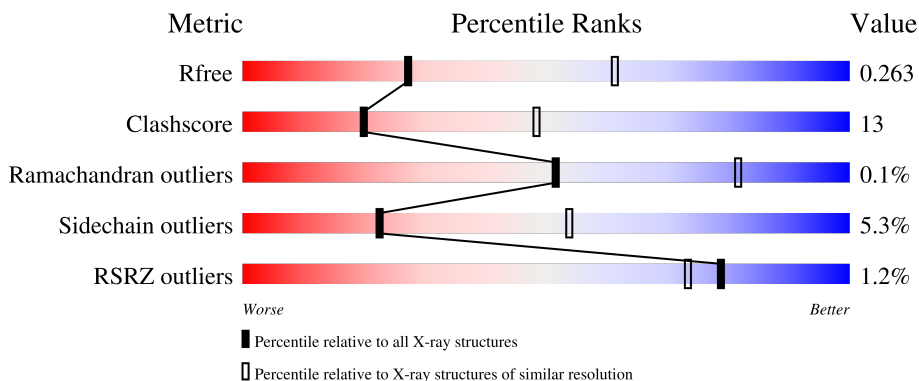
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




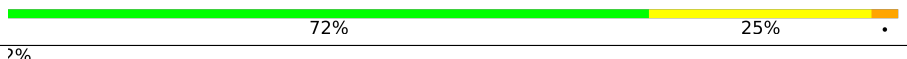
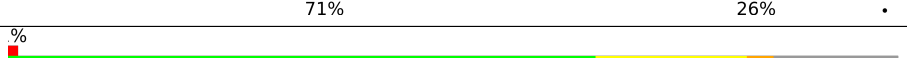
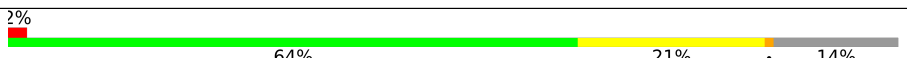
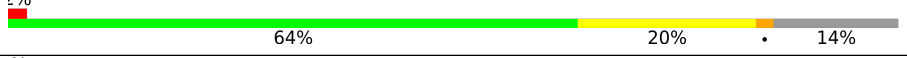

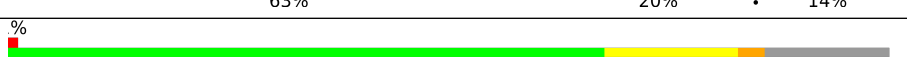


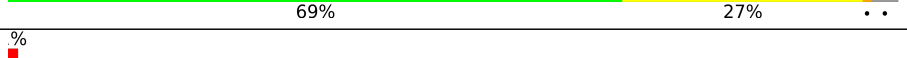
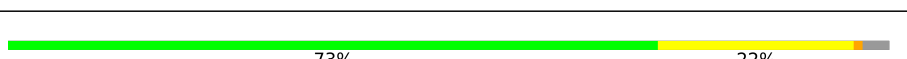


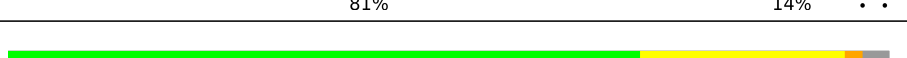
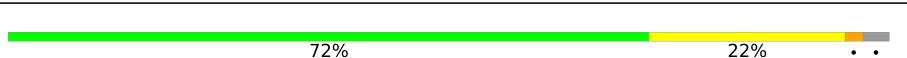
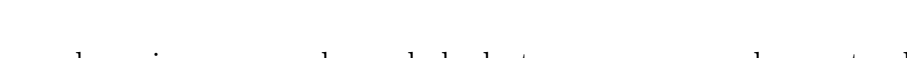
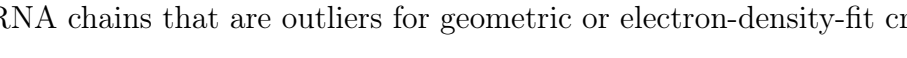
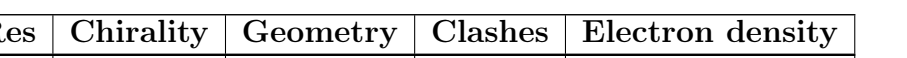
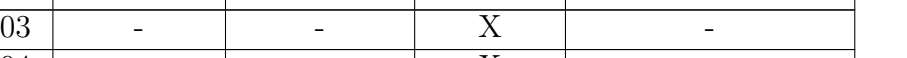
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	478	 71% 26% .
1	D	478	 72% 26% .
1	G	478	 76% 23% .
1	J	478	 73% 24% .
1	M	478	 76% 22% .

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Mol	Chain	Length	Quality of chain			
1	P	478		71%	26%	•
1	S	478		72%	25%	•
1	V	478		71%	26%	•
2	B	478		66%	17%	• 14%
2	E	478		64%	21%	• 14%
2	H	478		64%	20%	• 14%
2	K	478		64%	19%	• 14%
2	N	478		63%	20%	• 14%
2	Q	478		67%	15%	• 14%
2	T	478		65%	19%	• 14%
2	W	478		65%	18%	• 14%
3	C	94		69%	27%	• •
3	F	94		73%	21%	• •
3	I	94		73%	22%	• •
3	L	94		77%	19%	• •
3	O	94		76%	20%	• •
3	R	94		81%	14%	• •
3	U	94		71%	23%	• •
3	X	94		72%	22%	• •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GLN	A	901	-	-	X	-
4	GLN	G	903	-	-	X	-
4	GLN	J	904	-	-	X	-
4	GLN	M	905	-	-	X	-
4	GLN	P	906	-	-	X	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	GLN	V	908	-	-	X	-
5	MG	W	479	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 62935 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	478	3784	2450	615	712	7	0	0	0
1	D	478	3784	2450	615	712	7	0	0	0
1	G	478	3784	2450	615	712	7	0	0	0
1	J	478	3784	2450	615	712	7	0	0	0
1	M	478	3784	2450	615	712	7	0	0	0
1	P	478	3784	2450	615	712	7	0	0	0
1	S	478	3784	2450	615	712	7	0	0	0
1	V	478	3784	2450	615	712	7	0	0	0

- Molecule 2 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	410	3308	2104	567	622	15	0	0	0
2	E	410	3308	2104	567	622	15	0	0	0
2	H	410	3308	2104	567	622	15	0	0	0
2	K	410	3308	2104	567	622	15	0	0	0
2	N	410	3308	2104	567	622	15	0	0	0
2	Q	410	3308	2104	567	622	15	0	0	0

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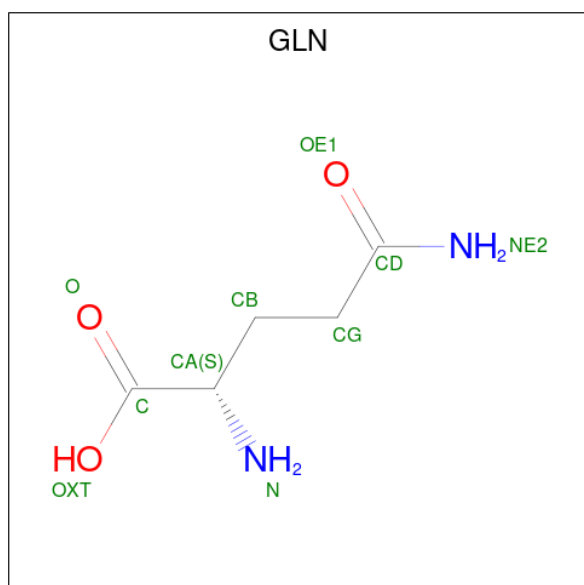
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	W	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			

- Molecule 3 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	F	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	I	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	L	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	O	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	R	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	U	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	X	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			

- Molecule 4 is GLUTAMINE (three-letter code: GLN) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	5	1	3		
4	D	1	Total	C	N	O	0	0
			9	5	1	3		
4	G	1	Total	C	N	O	0	0
			9	5	1	3		
4	J	1	Total	C	N	O	0	0
			9	5	1	3		
4	M	1	Total	C	N	O	0	0
			9	5	1	3		
4	P	1	Total	C	N	O	0	0
			9	5	1	3		
4	S	1	Total	C	N	O	0	0
			9	5	1	3		
4	V	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		
5	N	1	Total	Mg	0	0
			1	1		
5	Q	1	Total	Mg	0	0
			1	1		
5	T	1	Total	Mg	0	0
			1	1		
5	W	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		
6	E	1	Total	Zn	0	0
			1	1		
6	H	1	Total	Zn	0	0
			1	1		

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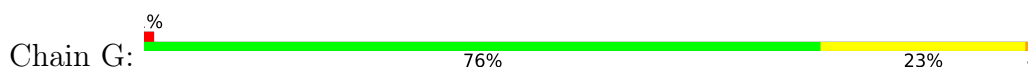
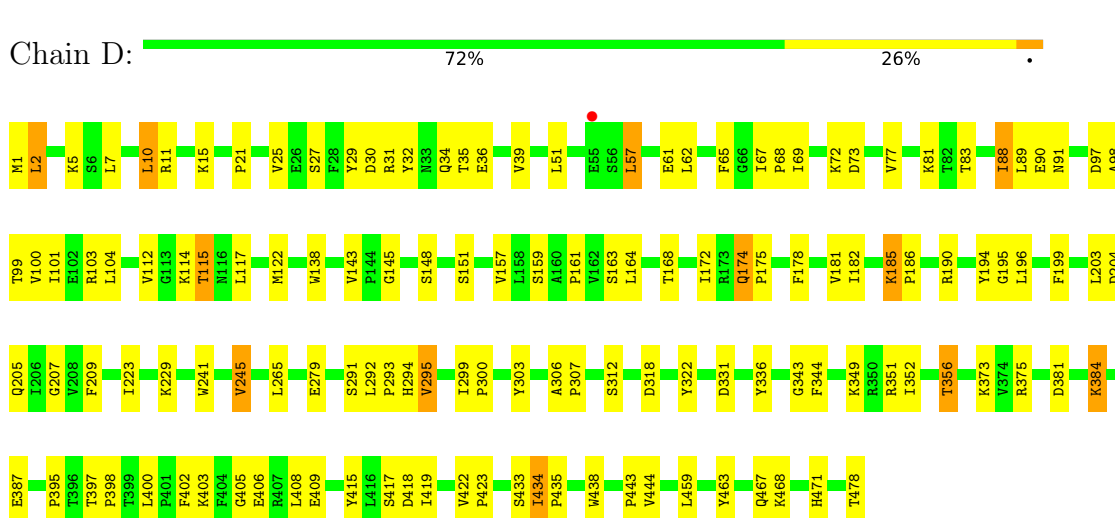
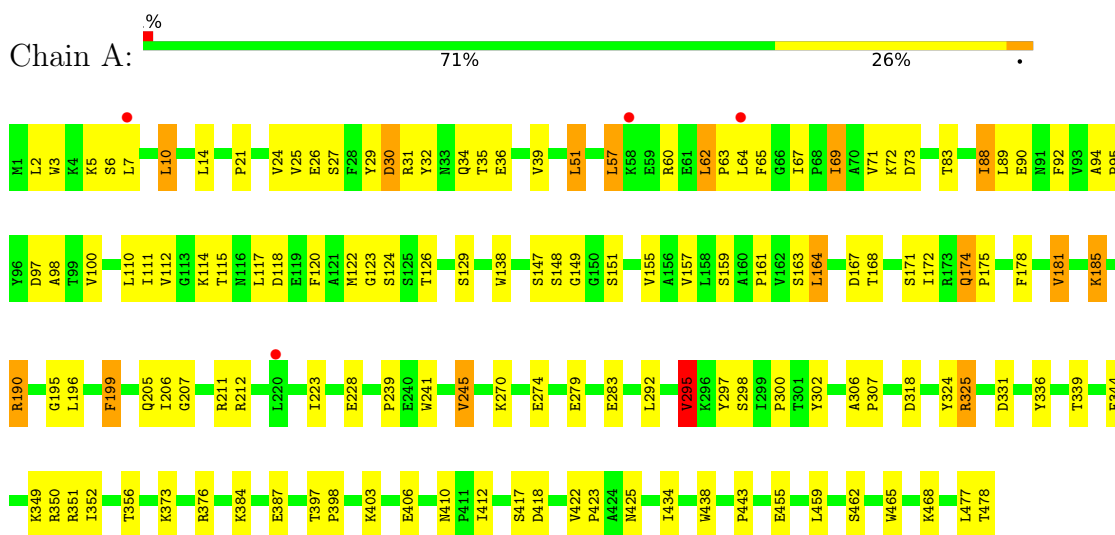
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	K	1	Total 1	Zn 1	0	0
6	N	1	Total 1	Zn 1	0	0
6	Q	1	Total 1	Zn 1	0	0
6	T	1	Total 1	Zn 1	0	0
6	W	1	Total 1	Zn 1	0	0

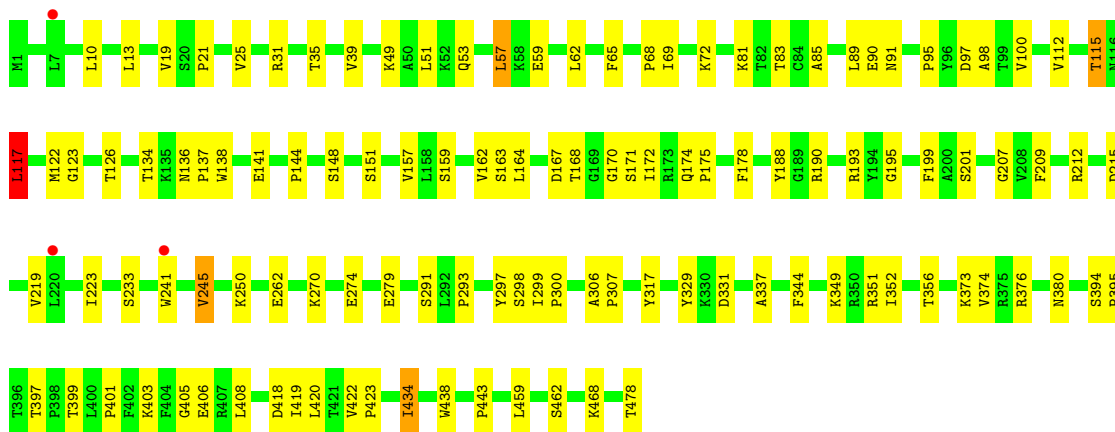


### 3 Residue-property plots [i](#)

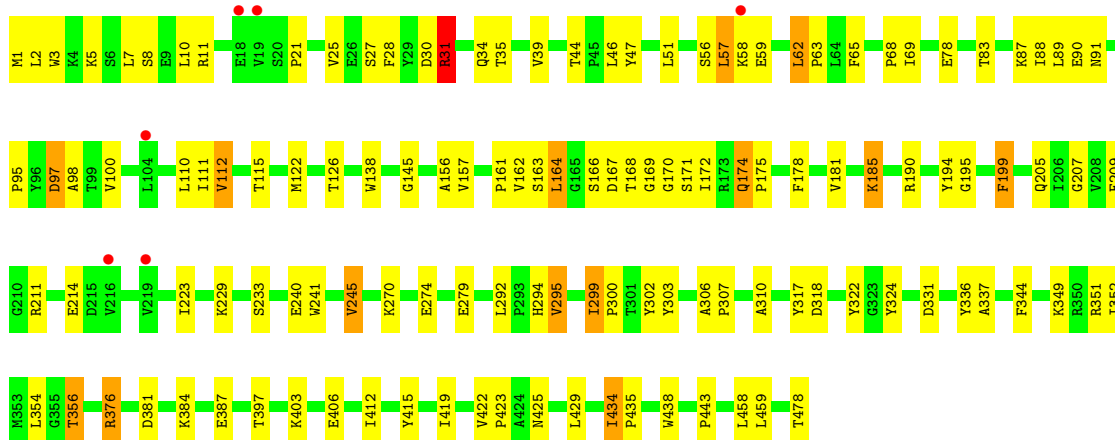
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

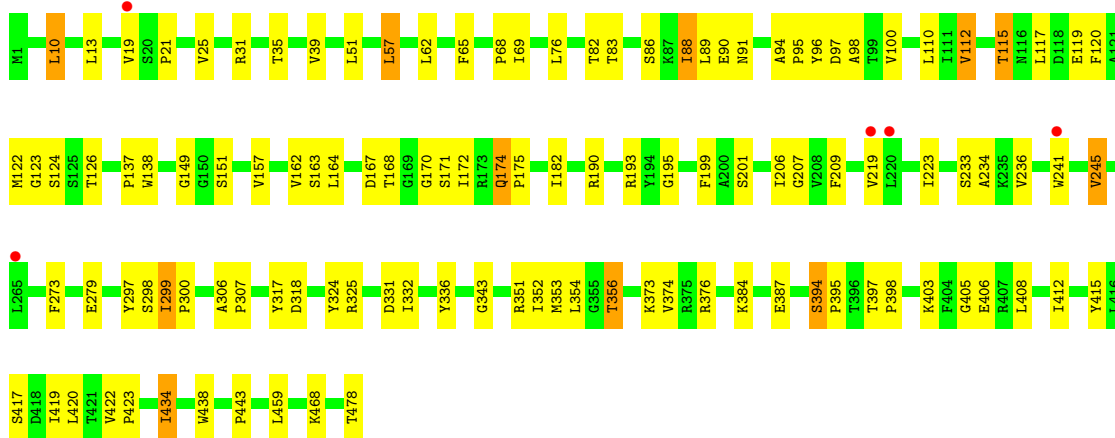
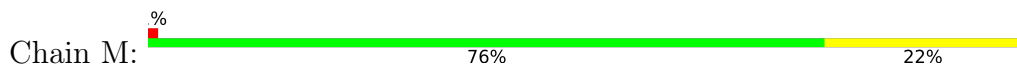




• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



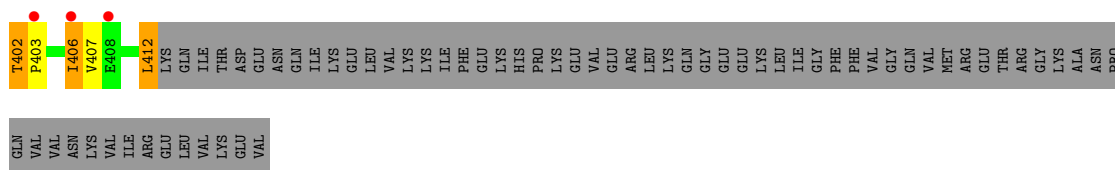
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



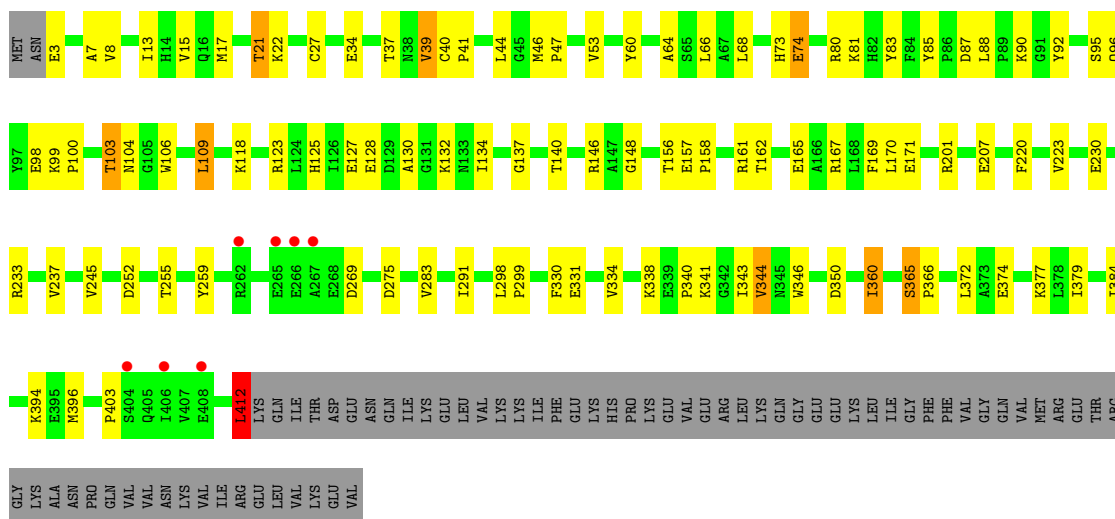
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



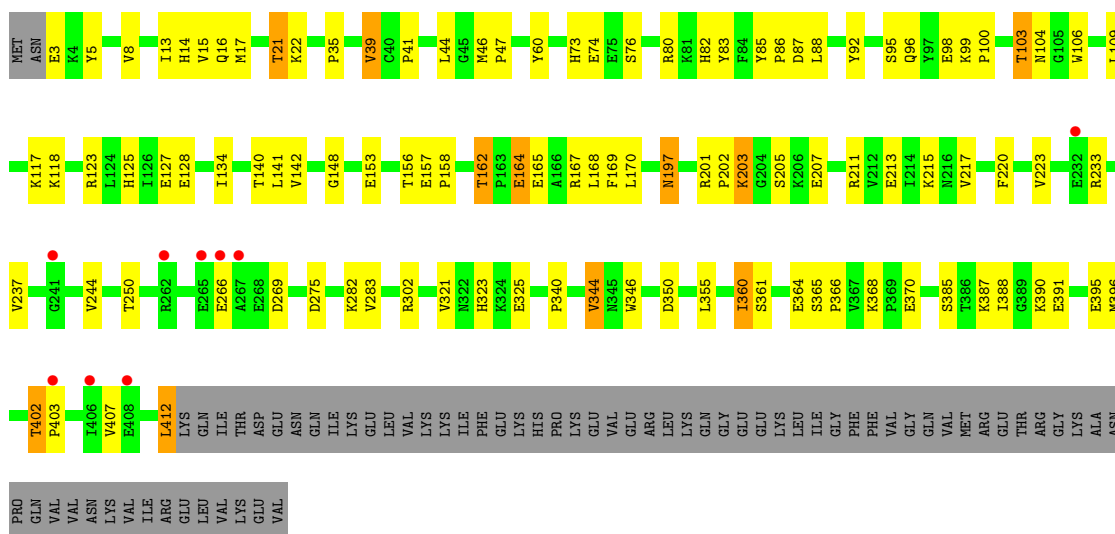




● Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

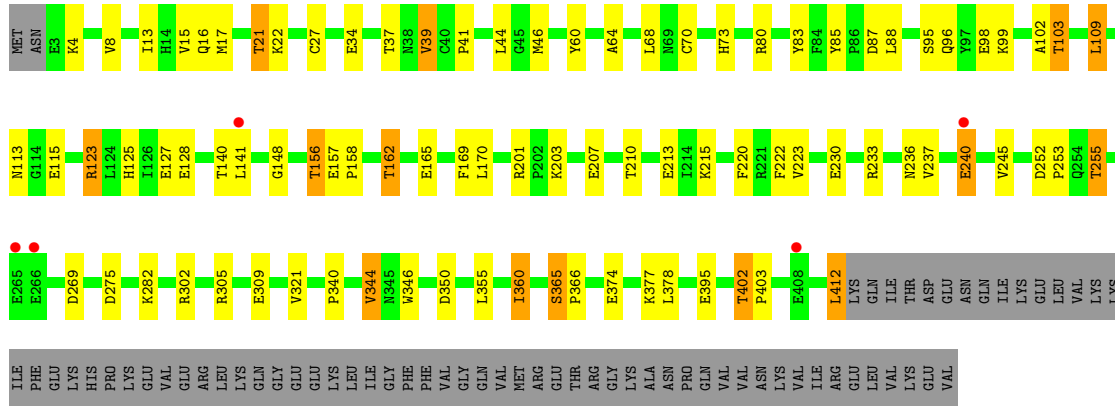


● Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

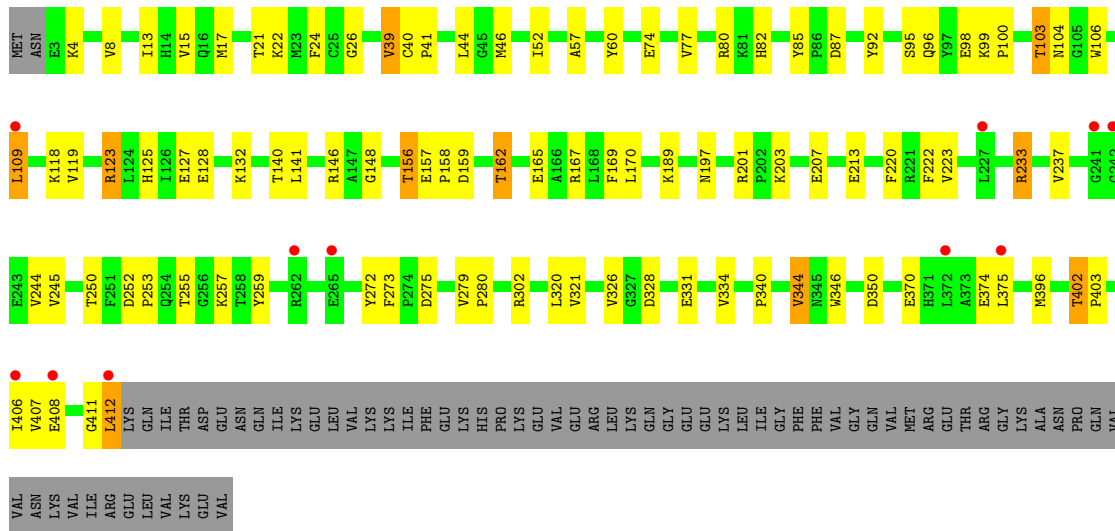


● Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

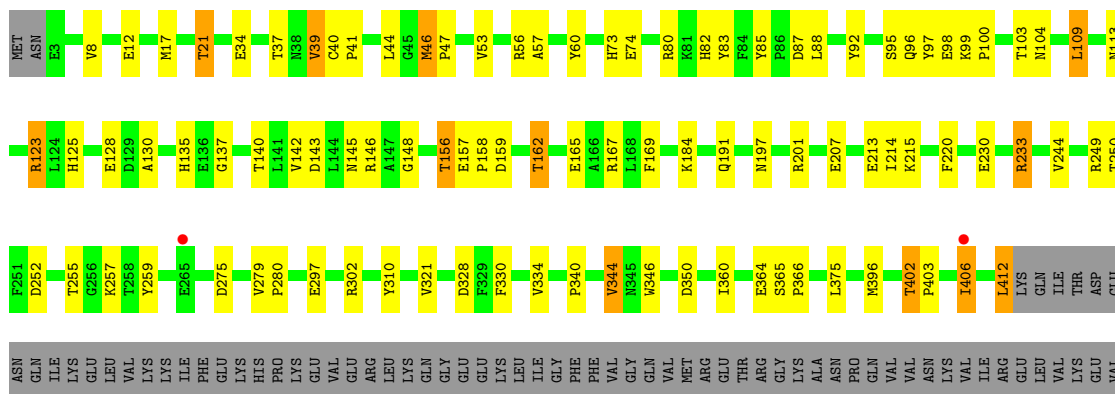




• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

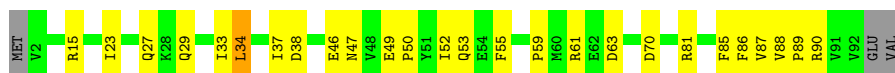


• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B




• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain C:  69% 27% ..



• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain F:  73% 21% ..




• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain I:  73% 22% ..




• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain L:  77% 19% ..




• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain O:  76% 20% ..



• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain R:  81% 14% ..



• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain U:  71% 23% ..



• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain X:  72% 22% ..





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.25Å 129.86Å 155.07Å 90.01° 89.96° 90.11°	Depositor
Resolution (Å)	39.37 – 2.80 39.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.37-2.80) 97.6 (39.36-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.254 , 0.305 0.260 , 0.263	Depositor DCC
$R_{free}$ test set	12256 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtrriage
Anisotropy	0.753	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 15.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.000 for -k,h,l 0.000 for k,-h,l 0.185 for h,-k,-l 0.437 for -h,k,-l 0.184 for -h,-k,l 0.000 for -k,-h,-l 0.000 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	62935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2523e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.64	0/3874	0.72	3/5244 (0.1%)
1	D	0.62	0/3874	0.70	2/5244 (0.0%)
1	G	0.62	0/3874	0.70	3/5244 (0.1%)
1	J	0.63	0/3874	0.70	3/5244 (0.1%)
1	M	0.61	0/3874	0.69	2/5244 (0.0%)
1	P	0.61	0/3874	0.69	2/5244 (0.0%)
1	S	0.63	0/3874	0.71	3/5244 (0.1%)
1	V	0.65	0/3874	0.72	2/5244 (0.0%)
2	B	0.59	0/3371	0.65	0/4541
2	E	0.61	1/3371 (0.0%)	0.64	0/4541
2	H	0.61	0/3371	0.65	1/4541 (0.0%)
2	K	0.61	0/3371	0.67	2/4541 (0.0%)
2	N	0.60	0/3371	0.67	2/4541 (0.0%)
2	Q	0.60	0/3371	0.68	2/4541 (0.0%)
2	T	0.62	0/3371	0.65	0/4541
2	W	0.59	0/3371	0.65	0/4541
3	C	0.58	0/778	0.71	0/1050
3	F	0.58	0/778	0.67	0/1050
3	I	0.56	0/778	0.69	0/1050
3	L	0.56	0/778	0.67	0/1050
3	O	0.56	0/778	0.71	0/1050
3	R	0.58	0/778	0.67	0/1050
3	U	0.60	0/778	0.70	0/1050
3	X	0.60	0/778	0.73	0/1050
All	All	0.61	1/64184 (0.0%)	0.68	27/86680 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1
2	B	0	2
2	E	0	2
2	T	0	1
3	F	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	43	CYS	CB-SG	-5.64	1.72	1.81

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	269	ASP	CB-CG-OD1	5.96	123.66	118.30
2	H	412	LEU	CA-CB-CG	5.92	128.92	115.30
1	J	31	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	G	117	LEU	CA-CB-CG	5.56	128.09	115.30
2	K	269	ASP	CB-CG-OD1	5.45	123.21	118.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	217	VAL	Peptide
2	B	411	GLY	Peptide
2	E	217	VAL	Peptide
2	E	97	TYR	Peptide
3	F	45	THR	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3784	0	3817	118	0
1	D	3784	0	3816	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3784	0	3817	100	0
1	J	3784	0	3816	110	0
1	M	3784	0	3817	108	0
1	P	3784	0	3816	118	0
1	S	3784	0	3817	116	0
1	V	3784	0	3817	120	0
2	B	3308	0	3353	95	0
2	E	3308	0	3353	91	0
2	H	3308	0	3353	82	0
2	K	3308	0	3353	77	0
2	N	3308	0	3353	71	0
2	Q	3308	0	3353	66	0
2	T	3308	0	3353	84	0
2	W	3308	0	3353	85	0
3	C	764	0	755	22	0
3	F	764	0	755	20	0
3	I	764	0	755	19	0
3	L	764	0	755	17	0
3	O	764	0	755	21	0
3	R	764	0	755	18	0
3	U	764	0	755	18	0
3	X	764	0	755	22	0
4	A	9	0	5	8	0
4	D	9	0	5	3	0
4	G	9	0	5	12	0
4	J	9	0	5	6	0
4	M	9	0	5	13	0
4	P	9	0	5	7	0
4	S	9	0	5	4	0
4	V	9	0	5	12	0
5	B	1	0	0	0	0
5	H	1	0	0	0	0
5	K	1	0	0	0	0
5	N	1	0	0	0	0
5	Q	1	0	0	0	0
5	T	1	0	0	0	0
5	W	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	H	1	0	0	0	0
6	K	1	0	0	0	0
6	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	1	0	0	0	0
6	T	1	0	0	0	0
6	W	1	0	0	0	0
All	All	62935	0	63437	1581	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 1581 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:LEU:HD22	2:B:412:LEU:O	1.39	1.22
1:P:464:LEU:HD12	1:P:464:LEU:O	1.40	1.20
3:O:88:VAL:HB	3:O:89:PRO:HD2	1.32	1.11
1:D:122:MET:HB3	1:D:351:ARG:NH1	1.63	1.11
2:T:412:LEU:O	2:T:412:LEU:HD22	1.49	1.11

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	476/478 (100%)	455 (96%)	20 (4%)	1 (0%)	47 78
1	D	476/478 (100%)	456 (96%)	18 (4%)	2 (0%)	34 66
1	G	476/478 (100%)	452 (95%)	23 (5%)	1 (0%)	47 78
1	J	476/478 (100%)	453 (95%)	23 (5%)	0	100 100
1	M	476/478 (100%)	453 (95%)	23 (5%)	0	100 100
1	P	476/478 (100%)	451 (95%)	24 (5%)	1 (0%)	47 78
1	S	476/478 (100%)	456 (96%)	20 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	476/478 (100%)	456 (96%)	18 (4%)	2 (0%)	34	66
2	B	408/478 (85%)	396 (97%)	12 (3%)	0	100	100
2	E	408/478 (85%)	390 (96%)	18 (4%)	0	100	100
2	H	408/478 (85%)	395 (97%)	13 (3%)	0	100	100
2	K	408/478 (85%)	392 (96%)	16 (4%)	0	100	100
2	N	408/478 (85%)	395 (97%)	13 (3%)	0	100	100
2	Q	408/478 (85%)	393 (96%)	15 (4%)	0	100	100
2	T	408/478 (85%)	388 (95%)	20 (5%)	0	100	100
2	W	408/478 (85%)	396 (97%)	12 (3%)	0	100	100
3	C	89/94 (95%)	86 (97%)	3 (3%)	0	100	100
3	F	89/94 (95%)	83 (93%)	6 (7%)	0	100	100
3	I	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	L	89/94 (95%)	86 (97%)	3 (3%)	0	100	100
3	O	89/94 (95%)	82 (92%)	7 (8%)	0	100	100
3	R	89/94 (95%)	83 (93%)	6 (7%)	0	100	100
3	U	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	X	89/94 (95%)	84 (94%)	4 (4%)	1 (1%)	14	41
All	All	7784/8400 (93%)	7451 (96%)	325 (4%)	8 (0%)	51	81

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	148	SER
1	A	148	SER
1	V	148	SER
1	D	2	LEU
1	D	148	SER

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/406 (100%)	383 (94%)	23 (6%)	20	50
1	D	406/406 (100%)	382 (94%)	24 (6%)	19	49
1	G	406/406 (100%)	391 (96%)	15 (4%)	34	68
1	J	406/406 (100%)	376 (93%)	30 (7%)	13	37
1	M	406/406 (100%)	387 (95%)	19 (5%)	26	59
1	P	406/406 (100%)	377 (93%)	29 (7%)	14	39
1	S	406/406 (100%)	382 (94%)	24 (6%)	19	49
1	V	406/406 (100%)	385 (95%)	21 (5%)	23	55
2	B	364/427 (85%)	345 (95%)	19 (5%)	23	55
2	E	364/427 (85%)	351 (96%)	13 (4%)	35	69
2	H	364/427 (85%)	347 (95%)	17 (5%)	26	59
2	K	364/427 (85%)	350 (96%)	14 (4%)	33	67
2	N	364/427 (85%)	340 (93%)	24 (7%)	16	44
2	Q	364/427 (85%)	345 (95%)	19 (5%)	23	55
2	T	364/427 (85%)	346 (95%)	18 (5%)	25	57
2	W	364/427 (85%)	346 (95%)	18 (5%)	25	57
3	C	86/89 (97%)	81 (94%)	5 (6%)	20	50
3	F	86/89 (97%)	83 (96%)	3 (4%)	36	70
3	I	86/89 (97%)	80 (93%)	6 (7%)	15	40
3	L	86/89 (97%)	82 (95%)	4 (5%)	26	59
3	O	86/89 (97%)	80 (93%)	6 (7%)	15	40
3	R	86/89 (97%)	83 (96%)	3 (4%)	36	70
3	U	86/89 (97%)	79 (92%)	7 (8%)	11	33
3	X	86/89 (97%)	81 (94%)	5 (6%)	20	50
All	All	6848/7376 (93%)	6482 (95%)	366 (5%)	22	54

5 of 366 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	115	THR
1	S	245	VAL
1	P	199	PHE
2	Q	240	GLU
2	T	103	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	275	ASN
2	K	323	HIS
2	W	345	ASN
2	T	110	ASN
1	V	460	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 15 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	GLN	S	907	1	7,8,9	0.89	0	7,9,11	1.49	2 (28%)
4	GLN	A	901	1	7,8,9	1.08	1 (14%)	7,9,11	1.56	2 (28%)
4	GLN	M	905	1	7,8,9	0.93	0	7,9,11	1.70	2 (28%)
4	GLN	G	903	1	7,8,9	1.07	0	7,9,11	1.54	2 (28%)
4	GLN	D	902	1	7,8,9	0.96	0	7,9,11	1.19	2 (28%)
4	GLN	J	904	1	7,8,9	0.91	1 (14%)	7,9,11	1.35	2 (28%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GLN	P	906	1	7,8,9	1.08	1 (14%)	7,9,11	1.47	2 (28%)
4	GLN	V	908	1	7,8,9	1.14	1 (14%)	7,9,11	1.33	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLN	S	907	1	-	0/7/8/9	-
4	GLN	A	901	1	-	0/7/8/9	-
4	GLN	M	905	1	-	0/7/8/9	-
4	GLN	G	903	1	-	0/7/8/9	-
4	GLN	D	902	1	-	0/7/8/9	-
4	GLN	J	904	1	-	0/7/8/9	-
4	GLN	P	906	1	-	1/7/8/9	-
4	GLN	V	908	1	-	0/7/8/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	906	GLN	OXT-C	-2.37	1.22	1.30
4	V	908	GLN	OXT-C	-2.25	1.23	1.30
4	A	901	GLN	OXT-C	-2.24	1.23	1.30
4	J	904	GLN	OXT-C	-2.05	1.23	1.30

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	905	GLN	OXT-C-O	-3.61	115.89	124.09
4	P	906	GLN	OXT-C-O	-2.92	117.47	124.09
4	G	903	GLN	OXT-C-CA	2.84	123.07	113.38
4	S	907	GLN	OXT-C-O	-2.79	117.76	124.09
4	A	901	GLN	OXT-C-CA	2.68	122.50	113.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	906	GLN	OXT-C-CA-N

There are no ring outliers.

8 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	907	GLN	4	0
4	A	901	GLN	8	0
4	M	905	GLN	13	0
4	G	903	GLN	12	0
4	D	902	GLN	3	0
4	J	904	GLN	6	0
4	P	906	GLN	7	0
4	V	908	GLN	12	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	478/478 (100%)	-0.04	4 (0%) 86 81	23, 52, 78, 87	0
1	D	478/478 (100%)	-0.02	1 (0%) 95 94	23, 52, 78, 87	0
1	G	478/478 (100%)	0.07	3 (0%) 89 86	23, 51, 77, 87	0
1	J	478/478 (100%)	0.04	6 (1%) 77 72	23, 51, 77, 87	0
1	M	478/478 (100%)	0.10	5 (1%) 82 77	23, 51, 77, 87	0
1	P	478/478 (100%)	0.04	5 (1%) 82 77	23, 51, 77, 87	0
1	S	478/478 (100%)	-0.05	2 (0%) 92 91	23, 52, 78, 87	0
1	V	478/478 (100%)	-0.01	8 (1%) 70 63	23, 52, 78, 87	0
2	B	410/478 (85%)	0.12	4 (0%) 82 77	31, 61, 92, 111	0
2	E	410/478 (85%)	0.07	8 (1%) 65 56	31, 62, 92, 111	0
2	H	410/478 (85%)	0.12	11 (2%) 54 44	31, 61, 92, 111	0
2	K	410/478 (85%)	0.09	7 (1%) 70 63	31, 61, 92, 111	0
2	N	410/478 (85%)	0.09	9 (2%) 62 52	31, 62, 92, 111	0
2	Q	410/478 (85%)	0.09	5 (1%) 79 73	31, 61, 92, 111	0
2	T	410/478 (85%)	0.06	11 (2%) 54 44	31, 61, 92, 111	0
2	W	410/478 (85%)	0.09	2 (0%) 91 88	31, 61, 92, 111	0
3	C	91/94 (96%)	0.09	0 100 100	25, 58, 71, 75	0
3	F	91/94 (96%)	0.09	1 (1%) 80 75	25, 58, 70, 75	0
3	I	91/94 (96%)	-0.04	0 100 100	25, 58, 71, 75	0
3	L	91/94 (96%)	0.02	0 100 100	25, 58, 71, 75	0
3	O	91/94 (96%)	0.06	0 100 100	25, 58, 71, 75	0
3	R	91/94 (96%)	0.00	0 100 100	25, 58, 70, 75	0
3	U	91/94 (96%)	0.10	0 100 100	25, 58, 71, 75	0
3	X	91/94 (96%)	0.14	0 100 100	25, 58, 71, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	7832/8400 (93%)	0.05	92 (1%) 79 73	23, 55, 87, 111	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	266	GLU	4.4
2	T	408	GLU	4.3
2	H	262	ARG	4.2
2	N	262	ARG	4.1
2	E	262	ARG	4.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	H	479	1/1	0.28	0.34	61,61,61,61	1
5	MG	B	479	1/1	0.35	0.29	57,57,57,57	1
5	MG	W	479	1/1	0.53	0.41	75,75,75,75	1
5	MG	K	479	1/1	0.63	0.28	53,53,53,53	1
4	GLN	A	901	9/10	0.64	0.31	48,49,55,59	0
4	GLN	J	904	9/10	0.69	0.37	59,59,60,63	0
4	GLN	P	906	9/10	0.69	0.34	52,53,54,56	0
5	MG	Q	479	1/1	0.72	0.24	61,61,61,61	1
4	GLN	V	908	9/10	0.72	0.32	49,51,54,59	0
4	GLN	M	905	9/10	0.73	0.30	47,48,53,60	0
4	GLN	G	903	9/10	0.74	0.23	51,52,60,65	0
4	GLN	S	907	9/10	0.76	0.24	55,56,57,62	0
5	MG	N	479	1/1	0.76	0.32	86,86,86,86	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GLN	D	902	9/10	0.82	0.33	55,56,57,61	0
5	MG	T	479	1/1	0.84	0.25	60,60,60,60	1
6	ZN	T	907	1/1	0.95	0.19	49,49,49,49	0
6	ZN	W	908	1/1	0.95	0.19	50,50,50,50	0
6	ZN	B	901	1/1	0.97	0.22	49,49,49,49	0
6	ZN	E	902	1/1	0.98	0.18	59,59,59,59	0
6	ZN	N	905	1/1	0.99	0.18	47,47,47,47	0
6	ZN	Q	906	1/1	0.99	0.17	44,44,44,44	0
6	ZN	H	903	1/1	0.99	0.17	51,51,51,51	0
6	ZN	K	904	1/1	0.99	0.16	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.